Extended Summaries of IUPAC Technical Reports

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Chirality in synthetic agrochemicals: bioactivity and safety considerations

(Kurihara N, Miyamoto J, Paulson GD, Zeeh B, Skidmore MW, Hollingworth RM and Kuiper HA, *Pure Appl Chem* **69**:2007–2025 (1997)).
IUPAC Technical Report on Pesticides 37 International Union of Pure and Applied Chemistry, Chemistry and the Environment Division, Commission on Agrochemicals and the Environment

SUMMARY

Most synthetic agrochemicals with chiral structures are marketed as racemates, even though the desired biological activity may be derived from only one isomer. However, some synthetic agrochemicals such as pyrethroid insecticides, aryloxypropanoate herbicides and triazole fungicides are marketed as the most biologically active isomer. Numerous reports describing the relative biological activities, preparations and analyses of enantiopure agrochemicals are available. Some examples of how different enantiomers in racemates are selectively metabolized have also been reported. When agrochemicals have chiral structures, efforts should be made to define the mode of action, elucidate metabolic pathways and to define the human and environmental toxicity of each isomer. If there are large differences in the biological activities of individual enantiomers in racemates, it is desirable to develop and use only the isomer with the highest sought-after biological activity.

RECOMMENDATIONS

(1) Studies are needed to better define the mechanisms of toxicity and metabolism of individual isomers of chiral and pro-chiral agrochemicals in target and non-target organisms.
(2) Where one or more isomers in a mixture pose significant environmental or human health risks, then that isomer should be removed even where it contributes to the desired biological activity.
(3) Where an isomer does not have the desired biological activity, it is preferable to remove that isomer, if economically feasible, even if it does not pose a significant risk. The use of only the stereoisomer with the desired biological activity will reduce the total amount of chemicals introduced into the environment, and therefore it merits careful consideration.
(4) Better methods for production of enantiopure isomers (biotechnology, asymmetric synthesis and/or separation) are needed.

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Pesticide fate in tropical soils

(Racke KD, Skidmore M, Hamilton DJ, Unsworth JB, Miyamoto J and Cohen SZ, *Pure Appl Chem* **69**:1349–1371 (1997))
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SUMMARY

Pesticide use is an important component of agricultural and non-agricultural pest control in tropical areas. However, the fate of pesticides in tropical soils is not as well understood as in soils from temperate regions. Tropical soils defy easy generalizations, but they are typically very old soils characterized by year-round uniformity of temperature regime. Although only a few studies have directly compared pesticide fate in tropical and temperate soils, there is no evidence that pesticides degrade more slowly under tropical conditions. Laboratory studies in which soils have been held under standardized conditions reveal that pesticide degradation rates and pathways are comparable between tropical and temperate soils. However, field investigations of fate of pesticides in tropical soils indicate that dissipation occurs more rapidly, in some cases much more so, than for pesticides used under similar temperate conditions. The most prominent mechanisms for this acceleration in pesticide dissipation appear to be related to the effect of tropical climates, and would include increased volatility and enhanced chemical and microbial degradation rates on an annualized basis.

RECOMMENDATIONS

(1) *Continued investigations in tropical soils and environments*. Investigations on the fate and effects of pesticides in tropical soils, especially under tropical environmental conditions, should continue to be encouraged. Pesticide regulatory

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agencies for countries with a significant tropical area should encourage field validation and/or modelling rather than require additional laboratory studies as a means of obtaining the most useful and regionally specific information on pesticide fate in tropical soils.

(2) *Further comparisons of pesticide fate in tropical and temperate soils*. Additional comparisons of pesticide fate in tropical and temperate soils should be made with the same experimental design. Execution of laboratory and field protocols across tropical and temperate soils or areas, inasmuch as they contribute to assembly and validation of pesticide fate models with broad, international applicability, would be especially valuable.

(3) *Application of modelling to pesticide fate under tropical conditions*. Further attempts should be made to validate environmental fate models for application to simulation of pesticide dissipation and mobility under tropical conditions.

(4) *Publication of data re fate of pesticides in tropical soils*. Results of investigations on pesticide fate in tropical soils should be published in international, peer-reviewed journals whenever possible, to increase accessibility of the information and insight obtained. Published reports should contain sufficient experimental information and data analysis to answer questions related to efficacy and environmental safety, so as to allow comparison with results from temperate areas.

Optimum use of available residue data in the estimation of dietary intake of pesticides

(Hamilton DJ, Holland PT, Ohlin B, Murray WJ, Ambrus A, de Baptista GC and Kovacicova J, *Pure Appl Chem* **69**:1373–1410 (1997))

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SUMMARY

Prediction of pesticide residue intake in human diets is vital for approving the use of pesticides and for gaining official acceptance of pesticide residue levels which occur in food commodities in international trade. Estimates for pesticide residue levels likely to be present in food as consumed are derived from supervised pesticide residue trials, residue monitoring, pesticide metabolism and food processing studies. The results of properly conducted total diet studies should generally displace other estimates, but they do not cover all pesticides and, in particular, are not available for a pesticide at its initial registration. Information was compiled on the range of residues occurring in a set of supervised residue trials with identical application rate, number of applications and pre-harvest interval, but at different sites with various crop varieties, operators, equipment and cultural practices. Where there were eight or more trials in a set (one data point per trial) the median residue was commonly 20–40% of the maximum and 80–100% of the mean. The median was generally a good measure of the modal or most commonly occurring value. The median residue in the edible portion of the commodity in the supervised trials (supervised trials median residue, STMR) was chosen as the starting point for chronic dietary intake estimation. The residue definition for dietary intake purposes should include metabolites and degradates of toxicological concern. Dietary intake for acute effects is best related to residue levels in a single serving of a food, or at least the average residue level in servings of the food over a day or so. The maximum residue occurring in the edible portion is the preferred starting point for intake estimates for potential acute effects. Residue levels in prepared food are often much reduced when the raw commodity is subject to trimming, washing, cooking, milling and refining. Food preparation and processing studies provide the basic information on the reduced or increased levels of residues in passing from the raw agricultural commodity to a processed commodity. The mean or median processing factors for residues in processing studies are combined with the STMR to provide the STMR-P (supervised trials median residue – prepared and processed food). Examples of data evaluation for captan and parathion-methyl are included in the paper. Residue monitoring data for 17 common pesticides on raw agricultural commodities were assembled in terms of incidence of residue detection. Within certain criteria the incidence of residue detection can be taken as a measure of percentage of crop treated. The majority of cases showed less than 1% incidence of pesticide residues (median value 0.5%). The incidence of residue detection exceeded 10% in 25 cases of the 208 pesticide/commodity combinations examined. A worked example for dithiocarbamates on apples demonstrates how information from supervised trials, processing studies and residue incidence are combined. Eighteen recommendations are provided for estimating the level of pesticide residues likely to be present in food as consumed.

RECOMMENDATIONS

(1) Dietary intake estimations should make the best use of all available data. This is preferred to a tiered approach because it is more economical to evaluate all information at the time of the review than to revisit it later. Also, a tiered approach may give the impression of 'manipulating the estimates until a desired result is achieved'.

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